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an effective potential for the scattered particle. Such an assumption is probably valid at high energies but then, the wave function should contain terms which allow for excitation and thus a single term in the Hartree series would not be valid. At energies below excitation, the incident particle is moving sufficiently slowly compared with the motion of the bound electrons that one would expect the atomic electrons to be able to follow the motion of the scattered particle while it is in the vicinity of the atom.

Refinements on the one product scheme have been proposed by Seaton [6] and Temkin [7]. Seaton suggests that the total wave function be expanded as a series of terms consisting of solutions to the bound state problem with coefficients which depend on the coordinates of the scattered electron. However, since one can expect an infinite number of terms the series must be truncated in order to compute the coefficients. Having once computed the coefficients, there is no machinery for going back and improving the estimate of the bound state distortion. Temkin uses the adiabatic approximation to compute the distortion of the bound state. He assumes that the incident electron is moving so slowly that one can consider the atom to be in the field of a static charge. By means of perturbation theory he is able to compute a distorted bound state wave function which depends parametrically on the position of the incident particle. The bound state function is then used to average the Hamiltonian over the atomic electrons to provide a one particle Hamiltonian for the scattered particle. Again, this technique suffers from the disadvantage that it does not contain any machinery for improving the estimates of the bound state distortion.

Our aim has been to develop a method whereby the self-consistent features of the Hartree approach can be incorporated into a form for the wave function which will contain correlations and satisfy the asymptotic boundary conditions. We have accomplished this by adding a sum of products of one particle functions to a product of the unperturbed bound state wave function and a function which will have the proper asymptotic form for a scattered particle. By requiring the terms in the sum to vanish at large distances, we have been able to obtain a set of coupled differential equations for the one particle functions. We can show that these differential equations lead to an effective one-particle Hamiltonian for the scattered particle in which the potential is made up of a sum of induced multipole potentials. We can also show that with a suitable set of approximations, the equations reduce to the adiabatic approximation.

Although our ultimate goal is to apply these equations to the problem of electron scattering from atoms, we have restricted ourselves to the scattering of a positron by hydrogen. By so doing, we need not consider effects of exchange which must add an additional complication in the electron problem, and we have an exact bound state eigenfunction which we would not have for any other atom. Although there is no experimental data for positron scattering from hydrogen, Spruch and Rosenberg [8] have computed a lower bound on the zero energy scattering length which can be used to estimate the efficacy of the approximation. The problem has some practical significance in that the cross-sections for atomic scattering are necessary to compute reaction rates for positronium formation [9].

There are two previous theoretical treatments of the low energy scattering of positrons by hydrogen. One is by Spruch and Rosenberg [8] and

one by Massey and Moussa [10]. Spruch and Rosenberg have shown that the Kato [11] method may be applied to the positron-hydrogen problem, and will provide anupper bound on the scattering length at zero energy. They examined various classes of wave functions to find one which gave the lowest bound and they found that the effects of correlation were such as to make the atom on the whole attractive to the positron whereas the static model would predict a repulsive interaction. The application of this method to systems which have a bound state has not been accomplished at non-zero energies and so is of limited value for the electron-atom scattering problem. Massey and Moussa introduced the correlation in a phenomenological way. Thus, if one assumes the atom to be a polarizable medium, it will acquire an induced dipole moment in the field of a point charge. This dipole moment is proportional to the field which varies as $1/r^2$. The potential of a point charge in the field of a dipole varies as $1/r^2$ times the dipole moment. Thus, the induced dipole potential varies as $1/r^4$. Massey and Moussa construct a one particle Hamiltonian containing a potential with this asymptotic behavior and choose a trial wave function for use with a variational principle. One may object to their work on two grounds. The first is that there is no consistent argument leading to the introduction of such a potential and the second is that the trial wave function they choose does not have the form which a solution to the polarization potential problem should have [12]. They find that the atom, while more attractive than would be supposed from the static approximation, is on the whole repulsive.

In Section II we construct the approximate wave function and use the Kohn variational principle to obtain a set of differential equations for

positron scattering. In Section III we show that the approximation results in an induced multipole expansion and we make the approximation of reducing the series to the dipole term. The relationship between this approximation and the adiabatic approximation is demonstrated in Section IV. The results of a numerical calculation of s-wave scattering are presented in Section V.

II Formulation of the Problem

2.1 Form of the wave function.

We make the usual assumption that the proton has an infinite mass and write the Hamiltonian in Hartree units with $\hbar = m_e = m_p = e = 1$,

$$H = K_1 + K_2 - \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}} , \tag{2-1}$$

where

$$K_1 = -\frac{1}{2}\nabla_1^2,$$

and

$\vec{r}_1 \equiv$ electron coordinate

$\vec{r}_2 \equiv$ positron coordinate

The effects due to the electron spins are neglected. Since the particles are not identical, there are no complications due to the Pauli Principle.

We shall confine ourselves to energies below the first excitation potential of hydrogen so the boundary condition is

$$\Psi(\vec{r}_1,\vec{r}_2) \xrightarrow[r_2 \to \infty]{} \psi_{100}(\vec{r}_1)\left[e^{ikz} + f(\theta_2)\frac{e^{ikr_2}}{r_2}\right] \tag{2-2}$$

where $\psi_{100}(\vec{r}_1)$ is the ground state hydrogenic function and k is the wave number of the positron.

The incident particle may be assumed to be in a superposition of orbital angular momentum states characterized by the quantum numbers ℓ_2, m_2. Similarly, the bound particle may be assumed to be in a superposition of hydrogenic states characterized by the quantum numbers n, ℓ_1, m_1. Since the individual orbital angular momenta are not constants of this motion, it is more convenient

to use a representation in which the total wave function, $\Psi(\vec{r}_1,\vec{r}_2)$, is given by a superposition of eigenfunctions of the total angular momentum, $\Psi(L,M|\vec{r}_1,\vec{r}_2)$. Thus,

$$(2\text{-}3) \qquad \Psi(r_1,r_2) = \sum_{L,M} A_{L,M}\, \Psi(L,M|\vec{r}_1,\vec{r}_2)$$

where the $A_{L,M}$ are chosen to satisfy the boundary condition, (2-2). Since the interaction, $1/r_{12}$, does not mix states of different L,M, the $\Psi(L,M|\vec{r}_1,\vec{r}_2)$ may be computed independently.

The $\Psi(L,M|\vec{r}_1,\vec{r}_2)$ can be expanded as a series of hydrogenic states, $\psi_{n\ell_1m_1}(\vec{r}_1)$, which satisfy the equations

$$\psi_{n\ell_1m_1}(\vec{r}_1) = \frac{1}{r_1}\, u_{n\ell_1}(r_1) Y_{\ell_1m_1}(\Omega_1)$$

$$\left[K_1 - \frac{1}{r_1} - E_n\right]\psi_{n\ell_1m_1}(\vec{r}_1) = 0$$

$Y_{\ell m}(\Omega) \equiv$ spherical harmonic.

Thus,

$$(2\text{-}4) \quad \Psi(L,M|\vec{r}_1,\vec{r}_2) = \sum_{\ell_1,\ell_2,n} \sum_{m_1,m_2} C_{\ell_1\ell_2}(L,M;m_1,m_2)\psi_{n\ell_1m_1}(\vec{r}_1)\,\frac{1}{r_2} \times$$

$$\times\, G(L,\ell_1,\ell_2,n|r_2) Y_{\ell_2m_2}(\Omega_2)$$

$$= \sum_{\ell_1,\ell_2,n} \frac{1}{r_1r_2}\, u_{n\ell_1}(r_1) G(L,\ell_1,\ell_2,n|r_2) \mathcal{Y}^M_{L\ell_1\ell_2}(\Omega_{12}) \,.$$

The [13] $C_{\ell_1\ell_2}(L,M;m_1,m_2)$ are the Clebsch-Gordon coefficients, the radial functions $G(L,\ell_1,\ell_2,n|r_2)$ are defined by (2-4), and

$$(2\text{-}5) \qquad \mathcal{Y}^M_{L\ell_1\ell_2} = C_{\ell_1\ell_2}(L,M;m_1,m_2)Y_{\ell_1 m_1}(\Omega_1)Y_{\ell_2 m_2}(\Omega_2).$$

The $\mathcal{Y}^M_{L\ell_1\ell_2}$ are eigenfunctions of the total angular momentum. The eigenvalue, M, describes the orientation of the system in space and since the scattering is independent of this orientation, $G(L,\ell_1,\ell_2,n|r_2)$ is independent of M.

We are concerned with low energy scattering by a hydrogen atom in its ground state. The energy eigenvalues of hydrogen in Hartree units are

$$(2\text{-}6) \qquad E_n = -\frac{1}{2n^2} \quad , \; n = 1,2,\ldots .$$

If the atom is initially in state, E_n, the total energy, E, is

$$(2\text{-}7) \qquad E = \frac{k^2}{2} + E_n$$

where k is the wave number. We shall take n = 1 and, following Spruch [8], restrict ourselves to

$$k^2 < .5$$

so that excitation to states with $n > 1$ and pickup of the electron by the positron are excluded.

Thus, taking the limit of $\Psi(L,M|\vec{r}_1,\vec{r}_2)$ for large r_2, we see that all the G's must vanish except the coefficient of $u_{10}(r_1)$, $G(L,0,\ell_2,1|r_2)$. This coefficient has the asymptotic form

$$(2\text{-}8) \qquad G(L,0,L,n|r_2) \rightarrow \alpha_L \sin(kr_2 - \tfrac{L\pi}{2}) + \beta_L \cos(kr_2 - \tfrac{L\pi}{2}).$$

Note that $\ell_2 = L$ for $\ell_1 = 0$. The ratio β_L/α_L is real and is given by

$$(2\text{-}9) \qquad \frac{\beta_L}{\alpha_L} = \tan \eta_L$$

where η_L is the phase shift.

Let us now split off the $u_{l0}(r_1)$ term from $\Psi(L,M|\vec{r}_1,\vec{r}_2)$ in (2-4) and write

$$(2\text{-}10) \qquad \Psi(L,M|\vec{r}_1,\vec{r}_2) = \frac{1}{r_1 r_2} u_{l0}(r_1) G(L,0,L,l|r_2) \mathcal{Y}^M_{LoL}$$

$$+ \frac{1}{r_1 r_2} \sum_{\ell_1,\ell_2} \left[\sum_{n \neq l} u_{n\ell_1} G(L,\ell_1,\ell_2,n|r_2) \right] \mathcal{Y}^M_{L\ell_1\ell_2}$$

$$= \Psi_H(L,M|\vec{r}_1,\vec{r}_2) + \frac{1}{r_1 r_2} \sum_{\ell_1,\ell_2} W^L_{\ell_1\ell_2}(r_1,r_2) \mathcal{Y}^M_{L\ell_1\ell_2}.$$

Here, Ψ_H is the form of the wave function used in the static approximation and

$$(2\text{-}11) \qquad W^L_{\ell_1\ell_2}(r_1,r_2) = \sum_{n \neq l} u_{n\ell_1}(r_1) G(L,\ell_1,\ell_2,n|r_2) \ .$$

One can obtain an approximate solution to the scattering problem by taking a finite number of terms in the series defining $W^{L}_{\ell_1\ell_2}$ and requiring that the $\Psi(L,M|\vec{r}_1,\vec{r}_2)$ so defined satisfy the Hartree equations

$$(2\text{-}12) \qquad \int \frac{1}{r_1} u_{n\ell_1}(r_1) \mathcal{Y}^{M}_{L\ell_1\ell_2} [H-E] \Psi(L,M|\vec{r}_1,\vec{r}_2) d\vec{r}_1 d\Omega_2 = 0.$$

An alternative approximation which we propose is to replace the sum over n in $W^{L}_{\ell_1\ell_2}$ by a single term of the form

$$(2\text{-}13) \qquad W^{L}_{\ell_1\ell_2}(r_1,r_2) = v_{\ell_1}(L|r_1) y_{\ell_2}(L|r_2)$$

where the $v_{\ell_1}(L|r_1)$ and the $y_{\ell_2}(L|r_2)$ are to be determined by a variational calculation. If we think of $W^{L}_{\ell_1\ell_2}$ as a correction to the lowest order Hartree term, Ψ_H, then (2-13) may be thought of as a Hartree approximation for the correction. This approach suffers from the usual difficulty in that the correlations we obtain by summing over n are suppressed. On the other hand, the total wave function for given L,M is correlated.

We define our approximate wave function, Ψ_P, as

$$(2\text{-}14) \qquad \Psi_P(L,M|\vec{r}_1,\vec{r}_2) = \frac{1}{r_1 r_2} \Big\{ u_{l0}(r_1) G(L,0,L,1|r_2) + \sum_{j_1 j_2} v_{j_1}(L|r_1) y_{j_2}(L|r_2) \mathcal{Y}^{M}_{Lj_1j_2} \Big\} .$$

Note that the sum over j_1 and j_2 is restricted only by the condition

$$j_1 + j_2 \geq L \geq |j_1 - j_2| .$$

The boundary conditions on the $y_{j_2}(L|r_2)$ are

$$y_{j_2}(L|r_2) \longrightarrow 0 \qquad \begin{matrix} r_2 \to 0 \\ r_2 \to \infty \end{matrix}$$

$v_{j_1}(L|r_1)$ must vanish at the origin and be regular over all space.

The choice of functional form for $v_{j_1}(L|r_1)$ and $v_{j_2}(L|r_2)$ is still an open question. Massey and Moussa [10] and Spruch and Rosenberg [8] introduced analytic expressions for

$$\sum_{j_1 j_2} W^{L}_{j_1 j_2}(r_1, r_2) \mathcal{Y}^{M}_{L j_1 j_2}.$$

These expressions contained unknown constants which were determined by a variational principle. Such a procedure enabled them to include terms with an r_{12} dependence. Having defined $W^{L}_{j_1 j_2}(r_1, r_2)$ to be a product of one-particle functions, we are free to determine these functions by means of a variational principle.

2.2 Variational method.

In order to obtain differential equations for G, y_{j_2} and v_{j_1} we shall use a variational principle of the type introduced by Kohn [1]. We first simplify the notation. We shall suppress the explicit radial Dependence of G, v and y as well as the explicit L dependence of v and y. Then, we may write

$$G(L,0,L,1|r_2) \equiv G_L$$

$$v_{j_1}(L|r_1) \equiv v_{j_1}$$

$$y_{j_2}(L|r_2) \equiv y_{j_2}.$$

We may also write

$$u_{10}(r_1) \equiv u = 2r_1 e^{-r_1} .$$

With this notation, (2-14) becomes

$$(2\text{-}15) \qquad \Psi_P(L,M|\vec{r}_1,\vec{r}_2) = \Psi_P = \frac{1}{r_1 r_2}\left[u\, G_L \mathcal{Y}^M_{LoL} + \sum_{j_1 j_2} v_{j_1} y_{j_2} \mathcal{Y}^M_{Lj_1j_2}\right]$$

The first order variation in Ψ_P is defined by

$$(2\text{-}16) \qquad \delta\Psi_P = \frac{1}{r_1 r_2}\left[u\delta G_L \mathcal{Y}^M_{LoL} + \sum_{j_1 j_2} \left(\delta v_{j_1} y_{j_2} + v_{j_1} \delta y_{j_2}\right) \mathcal{Y}^M_{Lj_1j_2}\right]$$

and, as $r \to \infty$

$$\delta y_{j_2} \to 0$$

$$\delta v_{j_1} \to 0$$

$$(2\text{-}17) \qquad \delta G_L \to \delta\alpha_L \sin(kr - \tfrac{L\pi}{2}) + \delta\beta_L \cos(kr - \tfrac{L\pi}{2})$$

The first order variations given in (2-17) insure that the function, $\Psi_P + \delta\Psi_P$, will satisfy the boundary conditions.

We define the integral,

$$(2\text{-}18) \qquad I = \int \Psi_P^{*}(H-E)\Psi_P d\tau_1 d\tau_2,$$

and compute

$$(2\text{-}19) \qquad \delta I = \int \delta\Psi_P^{*}(H-E)\Psi_P d\tau_1 d\tau_2 + \int \Psi_P^{*}(H-E)\delta\Psi_P d\tau_1 d\tau_2$$

$$= \int \delta\Psi_P^{*}(H-E)\Psi_P d\tau_1 d\tau_2 + \int \delta\Psi_P(H-E)\Psi_P^{*} d\tau_1 d\tau_2 + \Delta_1$$

The remainder, Δ_1, arises from the integrations by parts which are necessary to bring

$$\int \Psi_P^{*}(H-E)\delta\Psi_P d\tau_1 d\tau_2 \text{ into } \int \delta\Psi_P(H-E)\Psi_P^{*} d\tau_1 d\tau_2 .$$

When these involve $u, v_{j_1}, y_{j_2}, \delta v_{j_1}$ and δy_{j_2} no remainder accrues owing to the vanishing of the boundary terms. The integrations by parts necessary to transpose G_L^{*} and δG_L are carried out by taking the limit of the integral

$$(2\text{-}20) \quad -\frac{1}{2}\int_0^R \frac{1}{r^2} G_L^{*} \frac{1}{r_2^2}\frac{d}{dr_2} r_2^2 \frac{d}{dr_2}\frac{\delta G_L}{r^2} r_2^2 \, dr_2 \int_0^\infty |u|^2 \, dr_1 \times$$

$$\times \int \mathcal{Y}_{LoL}^{M\,*} \mathcal{Y}_{LoL}^{M} \, d\Omega_1 d\Omega_2 =$$

$$= - \frac{1}{2} \int_0^R G_L^* \frac{d^2}{dr^2} \delta G_L dr$$

as $R \to \infty$. Integrating by parts twice leads to

$$(2\text{-}21) \quad - \frac{1}{2} \int_0^R G_L^* \frac{d^2}{dr^2} \delta G_L = - \frac{1}{2} \left[G_L^* \frac{d}{dr} \delta G_L - \delta G_L \frac{d}{dr} G_L^* \right]_{r=R}$$

$$- \frac{1}{2} \int_0^R \delta G_L \frac{d^2}{dr} G_L^* \, dr.$$

The last term of (2-21) supplies the desired transposition. The bracketed term may be evaluated in terms of the asymptotic forms. Thus, using (2-8) and (2-17), we have

$$(2\text{-}22) \quad \Delta_1 = - \frac{1}{2} \left[G_L^* \frac{d}{dr} \delta G_L - \frac{dG_L^*}{dr} \delta G_L \right]_R = - \frac{1}{2} k \left(\beta_L^* \delta \alpha_L - \alpha_L^* \delta \beta_L \right) .$$

Recalling that

$$\left(\frac{\beta_L}{\alpha_L} \right)^* = \left(\frac{\beta_L}{\alpha_L} \right) = \tan \eta_L ,$$

Δ_1 may be written as

$$(2\text{-}23) \quad \Delta_1 = - \frac{k}{2} \left[\tan \eta_L \, \delta(\alpha_L^* \alpha_L) - \delta(\alpha_L^* \beta_L) \right] .$$

We assume that δv_{j_1}, δy_{j_2} and δG_L are independent variations and we further assume tan η_L in (2-23) to be set at its correct value. Then,

$$(2\text{-}24) \qquad \delta I - \Delta_1 = \delta\left(I + \frac{k}{2}(\alpha_L^* \alpha_L \tan \eta_L - \alpha_L^* \beta_L)\right) = 0$$

if the coefficients of the independent variations δv_{j_1}, δy_{j_2}, δG_L and their complex conjugates vanish. This leads to the stationary expression for the tangent of the phase shift,

$$(2\text{-}25) \qquad I - \frac{k}{2} \alpha_L^* \beta_L = - \frac{k}{2} \alpha_L^* \alpha_L \tan \eta_L .$$

Requiring the coefficients to vanish leads to the equations defining v_{j_1}, y_{j_2} and G_L; i.e.

$$(2\text{-}26) \qquad \int \frac{1}{r_1} u \mathcal{Y}^{M^*}_{LoL} (H-E)\Psi_P d\tau_1 d\Omega_2 = 0$$

$$(2\text{-}27) \qquad \sum_{j_2} \int \frac{1}{r_2} y_{j_2}^* \mathcal{Y}^{M^*}_{Lj_1j_2} (H-E)\Psi_P d\Omega_1 d\tau_2 = 0$$

$$(2\text{-}28) \qquad \sum_{j_1} \int \frac{1}{r_1} v_{j_1}^* \mathcal{Y}^{M^*}_{LoL} (H-E)\Psi_P d\tau_1 d\Omega_2 = 0$$

and a similar set for the complex conjugates.

2.3 The differential equations

On performing the indicated integrations in (2-26,27,28) we have

$$(2\text{-}29)\qquad \left[K^{(L)} + V_H - \frac{k^2}{2}\right]G_L + \langle u|v_o\rangle\left[K^{(L)} + \frac{1}{r_2} - \frac{k^2}{2}\right]y_L$$

$$- \sum_{j_1 j_2} \langle u|R_{j_1}|v_{j_1}\rangle \langle \mathcal{Y}^M_{LoL}|P_{j_1}|\mathcal{Y}^M_{Lj_1j_2}\rangle\, y_{j_2}$$

$$(2\text{-}30)\qquad N_v^{(j_1)}\left[K^{(j_1)} - \frac{1}{r_1} - \frac{E_v^{(j_1)}}{2}\right]v_{j_1} - \sum_{j_2, j'_2, j'_1, \gamma} \langle y_{j_2}|R_\gamma|y_{j'_2}\rangle$$

$$\langle \mathcal{Y}^M_{Lj_1j_2}|P_\gamma|\mathcal{Y}^M_{Lj'_1j'_2}\rangle v_{j'_1} + \langle y_L\left|K^{(L)} + \frac{1}{r_2} - \frac{k^2}{2}\right|G_L\rangle u\delta_{j_1 o}$$

$$- \sum_{j_2} \langle y_{j_2}|R_{j_1}|G_L\rangle \langle \mathcal{Y}^M_{Lj_1j_2}|P_{j_1}|\mathcal{Y}^M_{LoL}\rangle u = 0$$

$$(2\text{-}31)\qquad N_y^{(j_2)}\left[K^{(j_2)} + \frac{1}{r_2} - \frac{E_y^{(j_2)}}{2}\right]y_{j_2} - \sum_{\gamma, j_1, j'_1, j'_2} \langle v_{j_1}|R_\gamma|v_{j'_1}\rangle$$

$$\langle \mathcal{Y}^M_{Lj_1j_2}|P_\gamma|\mathcal{Y}^M_{Lj'_1j'_2}\rangle y_{j'_2} + \langle v_o|u\rangle\left[K^{(L)} + \frac{1}{r_2} - \frac{k^2}{2}\right]G_L\,\delta_{j_2 L}$$

$$- \sum_{j_1} \langle v_{j_1}|R_{j_1}|u\rangle \langle \mathcal{Y}^M_{Lj_1j_2}|P_{j_1}|\mathcal{Y}^M_{LoL}\rangle G_L = 0$$

where

$$(2\text{-}32) \qquad K^{(j)} = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{j(j+1)}{2r^2} \ .$$

We may ignore the complex character of the radial functions since it enters only through a complex normalization on G_L and consequently may be cancelled out of the equations. Thus,

$$(2\text{-}33) \qquad \langle w|f|z\rangle = \int_0^\infty w^*(x)f(x,y)z(x)dx$$

$$= \int_0^\infty w(x)f(x,y)z(x)dx \ .$$

The integrations over $1/r_{12}$ are carried out by expressing $1/r_{12}$ as

$$(2\text{-}34) \qquad \frac{1}{r_{12}} = \sum_\gamma \frac{r_<^\gamma}{(r_>)^{\gamma+1}} P_\gamma(\cos\theta_{12}) = \sum_\gamma R_\gamma P_\gamma(\cos\theta_{12})$$

$$r_< = \begin{cases} r_1, & r_2 > r_1 \\ r_2, & r_2 < r_1 \end{cases}$$

which defines R_γ.

The angular integrations are represented by

$$(2\text{-}35) \qquad \langle \mathcal{Y}^{M}_{Lj_1j_2} | P_\gamma | \mathcal{Y}^{M}_{Lj_1'j_2'} \rangle = \int \mathcal{Y}^{M^*}_{Lj_1j_2} P_\gamma(\cos\theta_{12}) \mathcal{Y}^{M}_{Lj_1'j_2'} d\Omega_1 d\Omega_2 .$$

These coefficients have been tabulated by Seaton[6] for a number of values of j_1 and j_2. They are independent of M and vanish unless

$$(2\text{-}36) \qquad (-)^{j_1 + j_2} = (-)^{j_1' + j_2'}$$

$$(2\text{-}37) \qquad (-)^{j_1 + j_1' + \gamma} = 1$$

$$(2\text{-}38) \qquad j_2 + \gamma \geq j_2' \geq |j_2 - \gamma| .$$

Equations (2-36,37) are expressions of parity conservation and (2-38) means that states with different multipole symmetry cannot be mixed by a multipole of order lower than the difference between their orders or by an order higher than their sum. The $\mathcal{Y}^{M}_{Lj_1j_2}$ satisfy the orthogonality relation

$$(2\text{-}39) \qquad \langle \mathcal{Y}^{M}_{Lj_1j_2} | \mathcal{Y}^{M}_{Lj_1'j_2'} \rangle = \langle \mathcal{Y}^{M}_{Lj_1j_2} | P_o | \mathcal{Y}^{M}_{Lj_1'j_2'} \rangle = \delta_{j_1j_1'} \delta_{j_2j_2'} .$$

V_H is defined as

$$V_H = \frac{1}{r} - \sum_\gamma \langle u | R_\gamma | u \rangle \langle \mathcal{Y}^{M}_{LoL} | P_\gamma | \mathcal{Y}^{M}_{LoL} \rangle$$

which by (2-38) and (2-39) reduces to

$$(2\text{-}40) \qquad V_H = \frac{1}{r} - \langle u | R_o | u \rangle$$

$$= \frac{1}{r} - \frac{1}{r} \int_o^r u^2 \, dt - \int_r^\infty \frac{u^2}{t} \, dt$$

$$= e^{-2r} \left(\frac{1}{r} + 1 \right).$$

The constants E_v and E_y are defined by

$$(2\text{-}41) \qquad E_v^{(j_1)} = - 2 \sum_{j_2} \langle y_{j_2} | K^{(j_2)} + \frac{1}{r} - E | y_{j_2} \rangle \Big/ N_v^{(j_1)}$$

$$(2\text{-}42) \qquad E_y^{(j_2)} = - 2 \sum_{j_1} \langle v_{j_1} | K^{(j_1)} + \frac{1}{r} - E | v_{j_2} \rangle \Big/ N_y^{(j_2)}$$

$$E = \frac{1}{2}(k^2 - 1).$$

$$(2\text{-}43) \qquad N_v^{(j_1)} = \sum_{j_2} \langle y_{j_2} | y_{j_2} \rangle$$

$$(2\text{-}44) \qquad N_y^{(j_2)} = \sum_{j_1} \langle v_{j_1} | v_{j_1} \rangle .$$

The sums over j_2 in (2-41,43) are restricted by

$$L + j_1 \geq j_2 \geq |L - j_1| .$$

A similar restriction holds for the sum over j_1 in (2-42,44).

In general, E_v and E_y will not be eigenvalues of (2-30,31) and consequently the complementary functions of these equations will not satisfy the boundary conditions. Thus, v_{j_1} and y_{j_2} must be the particular integrals of (2-30,31). There is the possibility that for sufficiently large k, E_y will be positive and (2-31) will have a complementary function with the asymptotic form $\sin(\sqrt{E_y}\, r)$. Such a term must not be thought of as a possible way of introducing excitations since in general the solution to (2-30), particular integral or otherwise, will not be an eigenfunction of the hydrogen atom Hamiltonian.

III The Dipole Approximation

3.1 Behavior near the origin

The differential equations (2-29,30,31) and the boundary conditions,

$$
\begin{aligned}
& y_{j_2} \to 0 \quad , \quad r \to 0,\infty \\
& v_{j_1} \to 0 \quad , \quad r \to 0,\infty \\
& G_L \to \alpha_L \sin(kr - \tfrac{L\pi}{2}) + \beta_L \cos(kr - \tfrac{L\pi}{2}) \quad , \quad r \to \infty \\
& G_L \to 0, \quad r \to 0,
\end{aligned}
\tag{3-1}
$$

define an infinite set of v_{j_1}'s and y_{j_2}'s for each value of L. These equations must be reduced in number before a practical solution is possible. We shall accomplish this reduction by assuming that the most important contribution of

$$
W^{L}_{j_1 j_2} = v_{j_1} y_{j_2} \tag{3-2}
$$

to the phase shift is made in the region of large r_2. We shall then show that the leading term in

$$
\sum W^{L}_{j_1 j_2} y^{M}_{L j_1 j_2} \text{ is } W^{L}_{1L}
$$

and that this term gives rise to an effective induced dipole potential in the equation defining G_L, (2-29). This approach may be justified by observing that in the neighborhood of the origin the behavior of G_L is determined primarily by the homogeneous part of (2-29). To see this, we note that (Appendix I)

$$(3\text{-}3) \qquad \langle w|R_\gamma|z\rangle \rightarrow r^\gamma \langle w|\frac{1}{t^{\gamma+1}}|z\rangle \ , \ r \rightarrow 0 \ .$$

We use (3-3) to write equations (2-29,31) in the limit of small r. Thus,

$$(3\text{-}4) \qquad \left[K^{(L)} + V_H - \frac{k^2}{2} \right] G_L + \langle u|v_o\rangle \left[K^{(L)} + \frac{1}{r} - \frac{k^2}{2} \right] y_L$$

$$- \langle u| \frac{1}{t} |v_o\rangle y_L = 0$$

$$(3\text{-}5) \qquad N^{(L)} \left[K^{(L)} + \frac{1}{r} - \frac{E_y^{(L)}}{2} \right] y_L - \sum_{j_1} \langle v_{j_1}| \frac{1}{t} |v_{j_1}\rangle y_L$$

$$+ \langle v_o|u\rangle \left[K^{(L)} + \frac{1}{r} - \frac{k^2}{2} \right] G_L - \langle v_o| \frac{1}{t} |u\rangle G_L = 0.$$

Since $V_H \rightarrow \frac{1}{r} - 1$ the behavior of G_L near the origin is given by

$$(3\ 6) \qquad \left[K^{(L)} + \frac{1}{r} - \frac{k^2}{2} - \frac{N}{N - |\langle v_o|u\rangle|^2} \right] G_L = E' y_L$$

where E' is a constant. A similar equation for y_L can be derived. Thus, the forms of G_L and y_L in the neighborhood of the origin are determined by the singularity in $K^{(L)}$ or by the Coulomb repulsion if $L = 0$. In either case,

$$(3\text{-}7) \qquad G_L \sim \sum_n C_n \, r^{(n+L+1)} \ .$$

The coefficients, c_o and c_1, are independent of y_L or v_o, c_2 will depend on y_L and c_n, $n > 2$ will depend on y_j, $j \neq L$. Since the centrifugal potential, $[L(L+1)]/r^2$, and the Coulomb potential are repulsive, we may expect that the positron will not penetrate the atom too deeply and the correlation term,

$$\sum_{\ell_1 \ell_2} W^{L}_{\ell_1 \ell_2},$$

will not be important for small r_2.

3.2 Asymptotic behavior of y and v

When $r_1, r_2 \to \infty$ equations (2-30,31) take the form

$$\sum_j \left[\mathcal{L}^{(j)} \delta_{ij} + V_{ij} \right] w_j = H_i \tag{3-8}$$

where, for $w_j = y_j$,

$$\mathcal{L}^{(i)} = N_v^{(i)} \left[K^{(i)} - E_y^{(i)} \right] \tag{3-9}$$

$$V_{ij} = \sum_{j_1, j_1'} \langle v_{j_1} | R_1 | v_{j_1'} \rangle \langle y^{M}_{Lj_1 i} | P_1 | y^{M}_{Lj_1' j} \rangle \tag{3-10}$$

$$V_{ij} = V_{ji} \quad ; \quad V_{ij} = 0, \; i \neq j \pm 1 \tag{3-11}$$

$$H_i = \langle v_\ell | R_\ell | u \rangle \langle y^{M}_{L\ell_i} | P_\ell | y^{M}_{LoL} \rangle G_L \tag{3-12}$$

$$\ell = |L - i|. \tag{3-13}$$

When $w_j = v_j$, we have

$$(3\text{-}14) \qquad \mathcal{L}^{(i)} = N_v^{(i)} \left[K^{(i)} - E_v^{(i)} \right]$$

$$(3\text{-}15) \qquad V_{ij} = \sum_{j_2 j_2'} \langle y_{j_2} | R_1 | y_{j'_2} \rangle \langle y^M_{Lij_2} | P_1 | y^M_{Ljj'_2} \rangle$$

$$(3\text{-}16) \qquad V_{ij} = V_{ji} \; ; \; V_{ij} = 0 \; , \; i \neq j \pm 1$$

$$(3\text{-}17) \qquad H_i = \sum_{j_2} \langle y_{j_2} | R_i | G_L \rangle \langle y^M_{Lij_2} | P_i | y^M_{LoL} \rangle u \; .$$

Equations (3-9) thru (3-18) are obtained by taking the leading terms in each of the expressions making up (2-30,31) and only the lowest order terms have been kept in each element of the matrix, $\mathcal{L}^{(i)}\delta_{ij} + V_{ij}$. The case of $w_L = y_L$ requires special treatment and will be considered after the other cases.

We assume w_j to have the asymptotic form,

$$(3\text{-}18) \qquad w_j \rightarrow f_j(r) \, e^{\lambda r},$$

where $f_j(r)$ is an asymptotic series of the form,

$$(3\text{-}19) \qquad f_j = \sum_n C_n^{(j)} \, r^{(s_j - n)} \; .$$

Then

$$(3\text{-}20) \qquad \sum_j N^{(i)} \left[K^{(i)} - \frac{E^{(i)}}{2} \right] \delta_{ij} w_j \rightarrow - \frac{N^{(i)}}{2} (\lambda^2 + E^{(i)}) w_i = A^{(i)}$$

where we drop all terms which vanish faster than $r^{s_j} e^{\lambda r}$. Using (3-20), we rewrite (3-8) as

$$(3\text{-}21) \qquad \sum_j A_{ij} w_j = \sum_j \left[A^{(i)} \delta_{ij} + V_{ij} \right] w_j = H_i \ .$$

The matrix, A, is real and symmetric and may therefore be diagonalized by a similarity transformation. If we consider V_{ij} to be a first order term, then A is diagonalized to first order by the transformation,

$$(3\text{-}22) \qquad \sum B_{ij} A_{jk} \tilde{B}_{k\ell} = A^{(i)} \delta_{i\ell}$$

where

$$(3\text{-}23) \qquad B_{ij} = \delta_{ij} - \frac{V_{ij}}{A^{(j)} - A^{(i)}} \ .$$

The inverse matrix, A^{-1}, is obtained from

$$(3\text{-}24) \qquad A^{-1}_{ij} = \sum_{k,\ell} \tilde{B}_{ik} \frac{1}{A^{(k)}} \delta_{k\ell} B_{\ell j}$$

$$= \frac{1}{A^{(i)}} \delta_{ij} - \frac{V_{ij}}{A^{(i)} A^{(j)}} \ .$$

The solution to (3-21) is given by

$$(3\text{-}25) \qquad w_i = \sum_{j,k} A^{-1}_{ij} A_{jk} w_k = \sum_j A^{-1}_{ij} H_j$$

$$= \frac{1}{A^{(i)}} H_i - \sum \frac{V_{ij} H_j}{A^{(i)} A^{(j)}} .$$

The asymptotic behavior of v_{j_1} is given by substituting (3-17) into (3-25) and setting $i = j_1$, $w_{j_1} = v_{j_1}$. Then, we must have $\lambda = -1$ in (3-19) and

$$(3\text{-}26) \qquad v_{j_1} \rightarrow f_{j_1} e^{-r} .$$

The form of the series is not of importance. The case of $j_1 = 1$ is calculated in Appendix I.

Since v_{j_1} vanishes exponentially,

$$\langle v_{j_1} | R_1 | v_{j_1'} \rangle \xrightarrow[r \rightarrow]{} \frac{1}{r^2} \int_0^\infty v_{j_1} t \, v_{j_1'} \, dt = \frac{1}{r^2} \langle v_{j_1} | t | v_{j_1'} \rangle .$$

Thus, V_{ij}, as defined by (3-10), vanishes as $1/r^2$. From (3-12) we have $H_i = r H_{i\pm1}$ or $H_i = \frac{1}{r} H_{i\pm1}$. In either case,

$$(3\text{-}27) \qquad V_{ij} H_j \sim H_i/r \quad \text{or} \quad H_i/r^3$$

so that the second term on the right of (3-25) vanishes more rapidly than the first and we have for $i = j_2$, $w_{j_2} = y_{j_2}$,

$$(3\text{-}28) \qquad y_{j_2} \rightarrow \frac{1}{A^{(i)}} H_i .$$

In order to satisfy (3-28) we redefine w_j in (3-18). Thus, take

$$(3\text{-}29) \qquad y_{j_2} = f_{j_2}(r)\sin(kr - \tfrac{L\pi}{2}) + g_{j_2}(r)\cos(kr - \tfrac{L\pi}{2}).$$

With (3-29), we must take $\lambda = ik$, where $i = \sqrt{-1}$, in previous formulas. Thus

$$(3\text{-}30) \qquad A^{(j)} = -\frac{N^{(j)}}{2}\left(E_y^{(j_2)} - k^2\right)$$

and from (3-12,13,25,30)

$$(3\text{-}31) \qquad y_{L\pm\ell} \longrightarrow \frac{2}{r^{\ell+1}} \frac{\langle v_\ell | t^\ell | u \rangle}{N^{(L\pm\ell)}(E_y^{(L\pm\ell)} - k^2)} \langle y^M_{L\ell(L\pm\ell)} | P_\ell | y^M_{LoL} \rangle G_L$$

$$= \frac{Q_{|L\pm\ell|}}{r^{\ell+1}} G_L .$$

Comparing (3-31) with (3-29), we have

$$(3\text{-}32) \qquad C_{fo}^{(L\pm\ell)} = Q_{L\pm\ell} \ , \quad C_{go} = \tan\eta_L \, Q_{L\pm\ell} \ , \quad S_{L\pm\ell} = -(\ell + 1),$$

where

$$f_j(r) = \sum C_{fn} r^{(s_j - n)} \ , \quad g_j(r) = \sum C_{gn} r^{(s_j - n)} .$$

The case of $\ell = 0$ is complicated by an additional term appearing in H_L and by the asymptotic cancellation of the G_L/r term. Thus;

$$(3\text{-}33) \qquad H_L = \langle v_2|R_2|u\rangle \langle y^M_{L2L}|P_2|y^M_{LoL}\rangle G_L - \left[K^{(L)} - \frac{k^2}{2}\right]G_L$$

Let us write (2-31) in the limit as $r_2 \to \infty$ for $j_2 = L$. Thus

$$(3\text{-}34) \qquad N_y^{(L)}\left[K^{(L)} - \frac{E_y^{(L)}}{2}\right]y_L + \langle v_o|u\rangle\left[K^{(L)} - \frac{k^2}{2}\right]G_L$$

$$- \sum_j \frac{1}{r^{j+1}} \langle v_j|t^j|u\rangle \langle y^M_{LjL}|P_2|y^M_{LoL}\rangle G_L = 0.$$

In the sum over j, the term with $j = 1$ vanishes by the parity rule, (2-36), and the first non-vanishing term occurs for $j = 2$. If $L < 2$ all terms in the sum vanish because of the vector coupling rule, (2-38). In this case, (3-34) reduces to

$$(3\text{-}35) \qquad N_y^{(L)}\left[K^{(L)} - \frac{E_y^{(L)}}{2}\right]y_L + \langle v_o|u\rangle\left[K^{(L)} - \frac{k^2}{2}\right]G_L = 0.$$

From (2-29),

$$(3\text{-}36) \qquad \left[K^{(L)} - \frac{k^2}{2}\right]G_L = -\langle u|v_o\rangle\left[K^{(L)} - \frac{k^2}{2}\right]y_L$$

$$+ \sum_j \frac{1}{r^2}\langle u|t|v_1\rangle \langle y^M_{LoL}|P_1|y^M_{Llj}\rangle y_j = 0 .$$

Substituting (3-36) into (3-35) results in an equation of the form

$$(3\text{-}37) \qquad \left[K^{(L)} - E' \right] y_L = \frac{B_+ y_{L+1} + B_- y_{L-1}}{r^2} = \frac{C\, G_L}{r^4}$$

so that

$$(3\text{-}38) \qquad y_L \sim \frac{C}{\frac{k^2}{2} - E'} \frac{G_L}{r^4} .$$

The theory presented in this section could not be considered rigorous insofar as the treatment of the differential operator, K, is concerned. However, a more extensive treatment involving the Green's function for the system is not necessary since we need only the leading terms of the asymptotic series. If the values of y_{j_2} are inserted into (2-31), the dominant terms in the differential equation are just the ones chosen in $\mathcal{L}^{(1)}$ and V_{ij}. We may therefore claim that the solutions obtained above do not lead to any inconsistency.

3.3 Multipole potentials

The asymptotic form of y_{j_2} given in the previous section will now be used to determine which values of j_1 and j_2 make the largest contribution to the scattering. Let us first consider the case of y_L. Now,

$$(3\text{-}39) \qquad \left[K^{(L)} - \frac{k^2}{2} \right] y_L = \left[K^{(L)} - E' + (E' - \frac{k^2}{2}) \right] y_L$$

$$= \frac{C\, G_L}{r^4} + (E' - \frac{k^2}{2}) \frac{C\, G_L}{(\frac{k^2}{2} - E')r^4} + \mathcal{O}\left(\frac{1}{r^5}\right)$$

$$= \mathcal{O}\left(\frac{1}{r^5}\right)$$

so that using y_L in (2-29) contributes a term which vanishes as $1/r^5$ for the case of $L < 2$. All other y_{j_2} contribute terms which vanish as $1/[r^{2(\ell+1)}]$.

Substituting (3-31) into the last term of (2-29), we obtain

$$(3\text{-}40) \qquad \sum_{\pm\ell} \sum_{j} \langle u|R_j|v_j\rangle \langle y^M_{LoL}|P_j|y^M_{Lj\,|L\pm\ell|}\rangle y_{|L\pm\ell|}$$

$$\simeq \sum_{\pm\ell} \frac{Q_{|L\pm\ell|}}{r^{2(\ell+1)}} \langle u|t^\ell|v_\ell\rangle \langle y^M_{LoL}|P_\ell|y^M_{L\ell\,|L\pm\ell|}\rangle G_L$$

$$= \sum_{\ell+o} \frac{Z_\ell}{r^{2(\ell+1)}} G_L = V_M G_L .$$

The "potential"

$$V_M = \sum_{\ell\neq o} \frac{Z_\ell}{r^{2(\ell+1)}}$$

is a sum of induced multipole potentials. The leading term is given by $\ell = 1$ and

$$V_M \sim \frac{Z_1}{r^4} .$$

The induced quadrupole term, $\ell = 2$ supplies the first correction and it vanishes as $1/r^6$. Thus we drop all $\ell > 1$.

When $L \geq 2$, y_L can contribute a term to (2-29) which vanishes as G_L/r^4 which arises from the term dropped from (3-34). Q_L would therefore be proportional to

$$(3\text{-}41) \qquad \langle v_2|t^2|u\rangle \ , \quad L \geq 2.$$

It is shown in the appendix that $v_j \to r^{j+1}$ in the neighborhood of the origin. Thus, as j increases, the first maximum of v_j moves out from the origin and consequently the overlap of v_j and u can be expected to decrease with increasing j. Then, $\langle v_j | t^j | u \rangle$ will decrease with increasing j and since $Q_{L\pm\ell}$ is proportional to $\langle v_\ell | t^\ell | u \rangle$ we can expect

$$Q_{L\pm1} > Q_{L\pm\ell} , \quad \ell \neq 1.$$

If these estimates are correct, we find that the largest contribution of $W^{L}_{j_1 j_2}$ to the effective potential seen by the positron arises from $\ell = 1$, $j_2 = L \pm 1$. Making this choice for j_2 restricts us to a single value for j_1, $j_1 = 1$.

The asymptotic form of Ψ_P in this approximation is

$$(3\text{-}42) \qquad \Psi_P \longrightarrow \frac{1}{r_1 r_2}\left[u\, y^{M}_{LoL} + \frac{1}{r_2^2} v_1 \left(Q_{L+1}\, y^{M}_{L1\ L+1} + Q_{L-1}\, y^{M}_{L1\ L-1}\right)\right] G_L .$$

This result is in agreement with perturbation calculations performed by Bransden, Dalgarno, John and Seaton [12] and by Temkin [7].

By retaining only the terms for which $j_1 = 1$, $j_2 = L \pm 1$ we effectively assume that the most important distortion of the atom arises from the coupling introduced by the dipole term. By dropping y_L and v_o we imply that the spherical distortion of the atom which arises from the monopole term in the expansion of $1/r_{12}$ is less important. It should be noted that our argument for the unimportance of y_L hinged on the fact that the leading term of the inhomogeneity $\langle v_o | R_o | u \rangle G_L$ in (2-31) was cancelled at large distances by $\frac{1}{r^2}\langle v_o | u \rangle G_L$. If this had not

been the case, y_L would have had the asymptotic form

$$y_L \sim \frac{G_L}{r}$$

and the inhomogeneity in the equation defining G_L would have been of the form G_L/r^2. Of course, if the cancellation did not take place, the atom would have a net charge and the effects of the spherical correlation might be swamped by the Coulombic term.

The arguments which were presented here hinged largely on the form of v_{j_1} at small distances and on the form of y_{j_2} at large distances. If these arguments are valid, they supply some justification to our choice of $W^L_{\ell_1\ell_2}(r_1 r_2)$ in 2-13). Thus, the exact $W^L_{\ell_1\ell_2}$ is given by

$$(3\text{-}43) \qquad W^L_{\ell_1\ell_2} = \sum_n u_{n\ell_1} G(L, \ell_1, \ell_2, n|r_2).$$

In general, $u_{n\ell_1}$ behaves near the origin as

$$u^{(r_1)}_{n\ell_1} \longrightarrow c_n r_1^{\ell_1+1}.$$

So that for small r_1,

$$W^L_{\ell_1\ell_2} \xrightarrow[r_1 \to o]{} r_1^{\ell_1+1} \sum_n c_n G(L, \ell_1, \ell_2, n|r_2)$$

and if this is the only region of importance where the form of $W^L_{\ell_1\ell_2}$ is concerned, we are then justified in assuming

$$W^L_{\ell_1\ell_2} = v_{\ell_1}(r_1) y_{\ell_2}(r_2).$$

IV The Adiabatic Approximation

Temkin [7] obtains the adiabatic approximation by assuming that the atom is in a static field whose source is the incident particle. The static field is treated as a perturbation and a distorted bound state function is found which depends parametrically on the position of the incident particle. The total wave function is a product of this distorted bound state and a function which depends on the coordinates of the scattered particle. The total wave function as computed by Temkin for electron scattering from hydrogen is

$$(4\text{-}1) \qquad \Phi = \left[\psi_{100} - \frac{\epsilon(r_2,r_1)}{r_2^2} \frac{v_{AD}(r_1)}{r_1} \frac{P_1(\cos\theta_{12})}{(4\pi)^{1/2}} \right] \frac{G(\vec{r}_1)}{r_1}$$

where

$$\epsilon(r_2,r_1) = \begin{cases} 0 , & r_2 < r_1 \\ 1 , & r_2 > r_1 \end{cases}$$

$P_1(\cos\theta_{12}) \equiv$ Legendre Polynomial

$$v_{AD} = (2r^2 + r^3)e^{-r}$$

Now, (4-1) is strongly reminiscent of (3-42). Thus

$$(3\text{-}42) \qquad \Psi_P \xrightarrow[r_2 \to \infty]{} \frac{1}{r_1 r_2} \left[u\, \mathcal{Y}^M_{LoL} + \frac{1}{r_2^2} v(r_1) \sum_{j_2 = L \pm 1} Q_{j_2} \mathcal{Y}^M_{L1j_2} \right] G_L$$

$v(r_1) = v_1$

Equation (4-1) can be obtained from (3-42) by assuming that y_{j_2} is negligible for $r_2 < r_c$ where r_c is some cut-off radius and that for $r_2 > r_c$

$$(4\text{-}2) \qquad y_{j_2} = Q_{j_2} \frac{G_L}{r_2^2}$$

where

$$(4\text{-}3) \qquad Q_{j_2} = \frac{\langle v | r | u \rangle}{\langle v | K^{(1)} - \frac{1}{r} + \frac{1}{2} | v \rangle} \langle y^M_{Llj_2} | P_1 | y^M_{LoL} \rangle .$$

We must compute $v(r_1)$ for $r_1 < r_c$ and to do this we assume

$$(4\text{-}4) \qquad \langle y_{j_2} | \frac{1}{r^{\gamma+1}} | y_{j_2'} \rangle = 0 , \quad \gamma \geq 1.$$

Applying (4-4) to $E_v^{(1)}$ results in

$$(4\text{-}5) \qquad \frac{E_v^{(1)}}{2} = \frac{1}{2}$$

since

$$\left[K^{(j_2)} - \frac{k^2}{2} \right] y_{j_2} \sim \frac{1}{r} \frac{dy}{dr} .$$

The differential equation for v_1 is

$$(2\text{-}30) \qquad N_v^{(1)} \left[K^{(1)} - \frac{1}{r} - \frac{E_v^{(1)}}{2} \right] v - \sum_{j_2, \gamma, j_2'} \langle y_{j_2} | R_\gamma | y_{j_2'} \rangle \times$$

$$\times \; \langle \mathcal{Y}^{M}_{Llj_2} | P_\gamma | \mathcal{Y}^{M}_{Llj_2'} \rangle v \quad - \sum_{j_2} \langle y_{j_2} | R_1 | G_L \rangle \times$$

$$\times \; \langle \mathcal{Y}^{M}_{Llj_2} | P_1 | \mathcal{Y}^{M}_{LoL} \rangle u = 0.$$

By (4-4), we may drop the second term in (2-30) since we are interested in $r_1 < r_c$. The last term in (2-30) is reduced by (4-2). Thus

$$(4\text{-}6) \qquad \langle y_{j_2} | R_1 | G_L \rangle = r_1 \int_{r_c}^{\infty} y_{j_2} \frac{G_L}{r_2^2} dr_2 = \frac{r_1}{Q_{j_2}} \int_{r_c}^{\infty} y_{j_2} y_{j_2} dr_2$$

$$= \frac{r_1}{Q_{j_2}} \langle y_{j_2} | y_{j_2} \rangle \quad .$$

Substituting (4-6) and (4-3) into (2-30), we have

$$(4\text{-}7) \qquad \left[K^{(1)} - \frac{1}{r_1} + \frac{1}{2} \right] v = r_1 u \; \frac{\langle v | K^{(1)} - \frac{1}{r} + \frac{1}{2} | v \rangle}{\langle v | r | u \rangle}$$

or

$$(4\text{-}8) \qquad \left[\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1 \right] v = hru$$

where

$$(4\text{-}9) \qquad h = \frac{\langle v \left[\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1 \right] v \rangle}{\langle v | r | u \rangle} \quad .$$

Now, h is completely arbitrary since

$$Q_{j_2} = -\frac{2}{h} \langle y^M_{Llj_2} | P_1 | y^M_{LoL} \rangle$$

and, since the solution of (4-8) is directly proportional to h, the product, $v_1 y_{j_2}$, is independent of h. It is shown in Appendix I that the solution to (4-8) for h = -2 is

(4-10) $\quad v = v_{AD}.$

The coefficients $\langle y^M_{Llj_2} | P_1 | y^M_{LoL} \rangle$ are evaluated by Seaton [6]. Thus

$$(4\text{-}11) \qquad \langle y^M_{Llj_2} | P_1 | y^M_{LoL} \rangle = \begin{cases} \dfrac{\sqrt{L}}{\sqrt{3(2L+1)}}, & j_2 = L - 1 \\ \dfrac{-\sqrt{L+1}}{\sqrt{3(2L+1)}}, & j_2 = L + 1 \end{cases}$$

Let us consider the case of L = 0. Then, with h = -2,

$$(4\text{-}12) \qquad Q_{j_2} = -\frac{1}{\sqrt{3}}, \quad L = 0$$

and

$$(4\text{-}13) \qquad y^o_{oll} = \sum_{m_1, m_2} C_{ll}(0,0;m_1,m_2) Y_{lm_1} Y_{lm_2} =$$

$$= \sum_{m_1} C_{11}(0,0;m_1,-m_1) Y_{1m_1} Y_{1-m_1}$$

$$= \sum_{m_1} (-)^{m_1} C_{11}(0,0;m_1-m_1) Y_{1m_1}^{*}(\Omega_1) Y_{1m_1}(\Omega_2)$$

$$= -\frac{1}{\sqrt{3}} \frac{3}{4\pi} P_1(\cos\theta_{12}).$$

Thus

$$\Psi_P \longrightarrow \frac{1}{r_1 r_2}\left[u\, y^{o}_{ooo} + \frac{1}{r_2^2} v_{AD} \frac{1}{4\pi} P_1(\cos\theta_{12})\right] G_o$$

or

$$\Psi_P \longrightarrow \left[\psi_{1oo} + \frac{1}{r_2^2} \frac{v_{AD}}{r_1} \frac{P_1(\cos\theta_{12})}{(4\pi)^{1/2}}\right] \frac{G_o}{r_2(4\pi)^{1/2}} .$$

Comparing (4-14) with (4-1) we see that the equations are the same except for the difference in sign. This results from the fact that Temkin considers electrons while we have considered positrons.

The case of $L > 0$ cannot be examined without a more detailed description of the function $G(\vec{r}_2)$ in (4-1). It should be noted that one of the features of our method of calculation is that angular effects are treated systematically throughout the development of the theory. This is not the case with the adiabatic approximation as derived from perturbation theory.

We note that the derivation of v_{AD} is independent of L. Thus, we can use v_{AD} and Q_{j_2} to compute the last term in (2-29), the equation defining G_L.

We have

$$(2\text{-}29) \qquad \left[K^{(L)} + V_H - \frac{k^2}{2} \right] G_L - \sum_{j_2} \langle u|R_1|v_1\rangle \langle y^M_{LoL}|P_1|y^M_{Llj_2}\rangle y_{j_2} = 0.$$

Here, $j_2 = L \pm 1$. Now,

$$(4\text{-}15) \qquad \langle u|R_1|v_{AD}\rangle = \frac{1}{r^2}\int_0^r ut\, v_{AD}dt + r\int_r^\infty u\,\frac{1}{t^2}\,v_{AD}\,dt\ .$$

We note that v_{AD} is regular over all space and since it decays exponentially we may approximate (4-15) by

$$(4\text{-}16) \qquad \langle u|R_1|v_{AD}\rangle \xrightarrow[r\to\infty]{} \frac{1}{r^2}\ \langle u|r_1|v_{AD}\rangle = \frac{2.25}{r^2}\ .$$

Using (4-2), (4-11) and (4-16), we have

$$(4\text{-}17) \qquad \left[K^{(L)} + V_H - \frac{k^2}{2} \right] G_L - \frac{\alpha}{2}\frac{G_L}{r^4} = 0$$

$$\alpha = 4.5$$

for large r. The last term in (4-17) is an induced dipole polarization potential. The value, $\alpha = 4.5$, is a well known result for the polarizibility.

V Results and Discussion

5.1 Numerical results for s-wave scattering

Equations (2-29,30,31) were evaluated numerically for s-wave scattering at energies such that $0. \leq k \leq .6$. The dipole approximation was assumed which reduced y_{j_2} to the single function, y_1. With

$$\begin{aligned} G_o &= G \\ y_1 &= y \\ v_1 &= v \quad , \end{aligned} \tag{5-1}$$

we have

$$\left\{ \frac{d^2}{dr^2} - 2V_H + k^2 \right\} G = \frac{2}{\sqrt{3}} \langle u|R_1|v\rangle y \tag{5-2}$$

$$\left\{ \frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} + \frac{2}{N_v} \left[\langle y|R_o|y\rangle + \frac{2}{5}\langle y|R_2|y\rangle \right] + E_v \right\} v = \frac{2}{\sqrt{3}} \langle y|R_1|G_o\rangle u \tag{5-3}$$

$$\left\{ \frac{d^2}{dr^2} - \frac{2}{r^2} - \frac{2}{r} + \frac{2}{N_y} \left[\langle v|R_o|v\rangle + \frac{2}{5}\langle v|R_2|v\rangle \right] + E_y \right\} y = \frac{2}{\sqrt{3}} \langle v|R_1|u\rangle v \, . \tag{5-4}$$

The normalization of Ψ_P depends on the normalization chosen for G. For $k = 0$, G was assumed to have the form

$$(5\text{-}5) \qquad G \xrightarrow[r \to \infty]{} r + A_o,$$

where A_o is the negative of the scattering length. For $k \neq 0$, G was assigned the asymptotic form

$$(5\text{-}6) \qquad G \xrightarrow[r \to \infty]{} \sin kr + \tan \eta \cos kr.$$

In Table 1, we list the values of the phase shifts obtained by the self-consistent method and those found by Spruch and Rosenberg [8], and Massey and Moussa [10]. We also list under the heading "static model", the values that are obtained by setting $v = y = 0$ in (5-2). This data is displayed in Figure 1 where we have plotted $\tan \eta/k$ vs. k.

From Figure 1 we see that the self consistent method gives a positive phase shift for $k < 3.5$. At higher energies the phase shift becomes negative in agreement with the results of the Born approximation. Comparing this with the static model for which the phase shifts are always negative, we see that at sufficiently small energies, the effect of the correlation is to make the atom attractive to the positron. The results of Massey and Moussa [10] indicate that the addition of an ad hoc polarization potential into the Hamiltonian will not greatly increase the attractiveness of the potential. The values listed for Spruch and Rosenberg [8] are the negative of upper bounds on $\tan \eta/k$. Thus, in this context, they represent lower bounds. The values of $\tan \eta/k$ as given by the self-consistent model are less than these bounds and must therefore be considered to be in error.

FIGURE 1

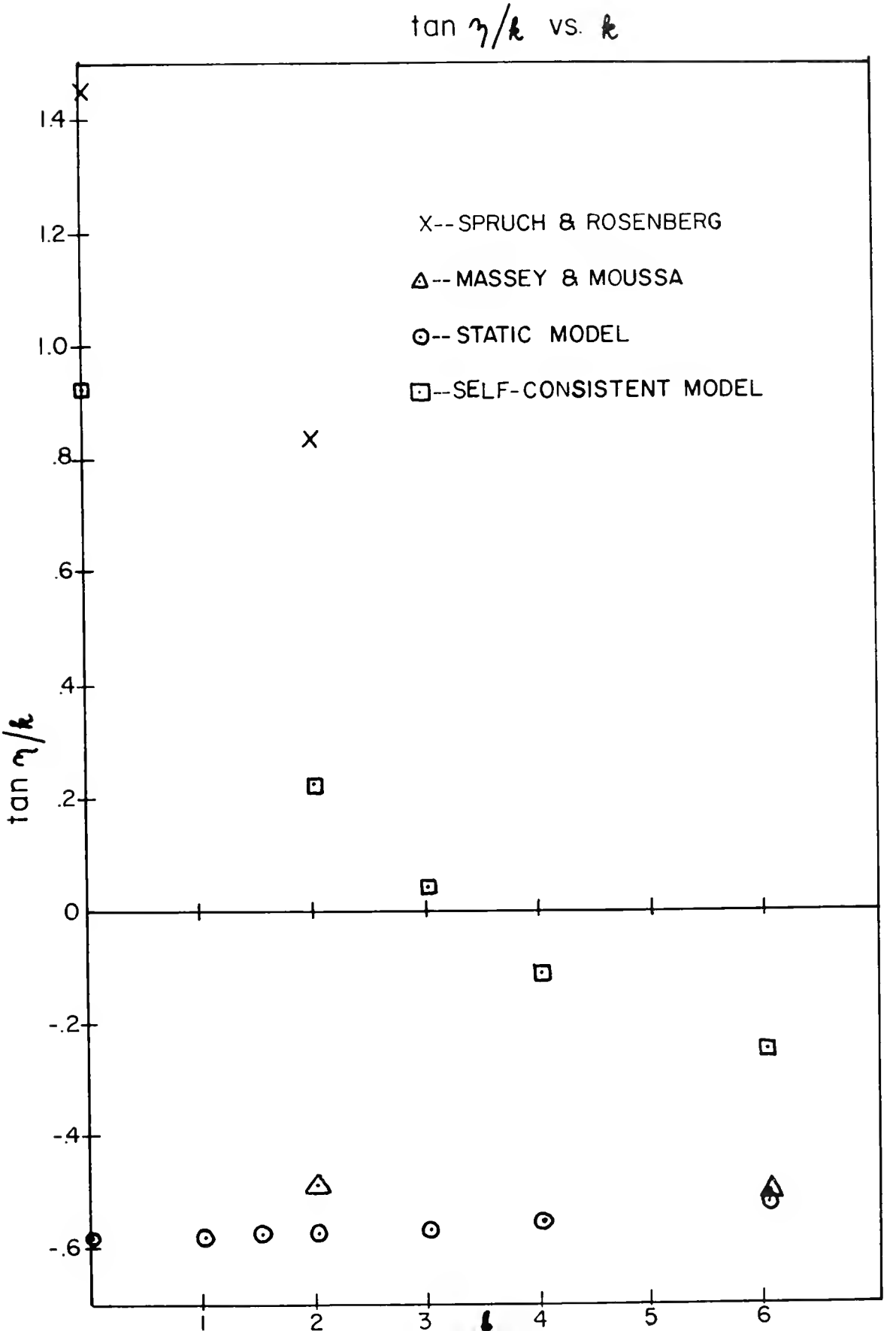
tan η/k vs. k
X--SPRUCH & ROSENBERG
△--MASSEY & MOUSSA
⊙--STATIC MODEL
⊡--SELF-CONSISTENT MODEL
tan η/k
1.4
1.2
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
1
2
3
4
5
6
k

TABLE 1.

k	SELF-CONSISTENT		STATIC MODEL		SPRUCH AND ROSENBERG [8]		MASSEY AND MOUSSA [10]	
	η	tan η/k	η	tan η/k	η	tan η/k	η	tan η/k
.0	-	.92	-	-.582	-	1.45	-	-
.2	.0451	.226	-.115	-.575	.156	.83	-.098	-.49
.3	.0109	.036	-.168	-.567	-	-	-	-
.4	-.0447	-.112	-.218	-.555	-	-	-	-
.5	-	-	-.264*	-.540*	-	-	-.251	-.508
.6	-.146	-.245	-.304	-.523	-	-	-	-

S-Wave Phase Shifts for Positron Hydrogen Scattering

k in units of a_o^{-1}

Our method gives substantially better results than the static approximation however.

For future reference, we list the values of the "constants" E_y, E_v, N_v and α in Table 2, where

$$E_y = \langle v | \frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1 + k^2 | v \rangle / \langle v | v \rangle$$

$$E_v = \langle y | \frac{d^2}{dr^2} - \frac{2}{r^2} - \frac{2}{r} - 1 + k^2 | y \rangle / \langle y | y \rangle$$

$$N_v = \langle y | y \rangle$$

and the polarizibility, α, is

$$\alpha = \frac{-2Q_1}{\sqrt{3}} \langle v | r | u \rangle$$

N_v for $k \neq 0$ cannot be compared directly with its value for $k = 0$. In order to find comparable values we must compute $\sqrt{N_v/k^2}$ for $k \neq 0$. This is necessary since the normalization of yv is proportional to the normalization of G and (5-5) is equivalent to

(5-7) $$\frac{1}{k} [\sin kr + \tan \eta \cos kr]$$

in the limit of vanishing k. The relative normalization of v and y is arbitrary and, in order to simplify the numerical work, the normalization of v was chosen such that

$$N_y = \langle v | v \rangle = \langle v_{AD} | v_{AD} \rangle = 16.125.$$

TABLE 2.

k in units of a_o^{-1}

k	E_y	E_v	N_v	$\frac{1}{k}\sqrt{N_v}$	α
0.	-.89	-1.5	.11	.33	4.4
.2	-.9	-1.8	$1.9\ 10^{-3}$	.22	4.3
.3	-.88	-1.9	$2.8\ 10^{-3}$	.18	4.
.4	-.84	-2.0	$3.4\ 10^{-3}$	.15	3.9
.6	-.72	-2.1	$4.2\ 10^{-3}$	.11	3.6

Static value of $\alpha = 4.5$

$N_y = 16.125$

$$E_y \equiv \langle v|\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1 + k^2|v\rangle / \langle v|v\rangle$$

$$E_v \equiv \langle y|\frac{d^2}{dr^2} - \frac{2}{r^2} - \frac{2}{r} - 1 + k^2|y\rangle / \langle y|y\rangle$$

$$N_v \equiv \langle y|y\rangle$$

5.2 Discussion of results

We see from Figure 1 that our self-consistent model is capable of explaining a large part of the attractive nature of the hydrogen-positron interaction as found by Spruch and Rosenberg [8]. There is reason to expect that extending the calculation to include spherical distortions would improve the phase shifts relative to Spruch's results. We base this on the following considerations:

From Table 2, it is seen that the values of α decrease much more slowly with increasing energy than does the phase shift. This suggests that the effective long tailed potential $\alpha G/r^4$ does not play a dominant role in determining the cross section. On the other hand, the values of

$$\frac{1}{k}\sqrt{N_v} = \sqrt{\langle y|y\rangle}\ /k$$

show a very precipitous decline. Now, $\langle v|v\rangle$ is independent of energy and consequently the normalization of y, $\frac{1}{k}\sqrt{N_v}$, is a measure of the importance of the correlation term. This indicates that the strong attraction at low energies are not due so much to the long tail of the effective potential as to effects of the correlation at smaller distances. In Section 3 we argued that we should retain only the dipole term since this makes the largest contribution at large r; but our results indicate that the most important part of the interaction may be due to the short range part of the correlation. For this reason we feel that the spherical distortion may contribute significantly even though it falls off more rapidly than the dipole term.

The experience of Massey and Moussa [10] lends some credence to this idea that short range effects predominate. They introduced a long tailed potential into a variational principle but they used a relatively uncorre-

lated wave function in comparison to the one chosen by Spruch and Rosenberg [8]. Despite the inclusion of polarization, the Massey and Moussa results indicate an overall repulsion only slightly less than that given by the static model.

The other argument which indicates the relative insensitivity of the phase shift to the long tailed potential is obtained from the solutions to (5-2,4) when v is chosen to be v_{AD}. In this case, $\alpha = 4.5$, but the value of tan η/k for zero energy is .85 as compared to .92 and a value of $\alpha = 4.4$ when the full iteration scheme is used.

It should be noted that the relative success of v_{AD} in predicting a value of tan η/k so close to the value obtained by solving (5-1) for v does not necessarily mean that the adiabatic theory will give similar results since the form of y is given by QG/r^2 only for large values of r. On the other hand, the numerical work involved in the self consistent model is considerably simplified with the choice of $v = v_{AD}$ and, since the difference between the results is small, it would probably be better in future applications to take this choice.

In this paper we have developed a self consistent Hartree model for the scattering of positrons by atoms and applied it to the scattering of positrons by hydrogen. The results of this application are encouraging since it seems possible to find by this method the distortion of the atoms by the slow incoming particle. This distortion plays a predominant role in this problem and may be important for more complicated problems.

While other techniques, especially the work of Spruch and Rosenberg, have previously shown the importance of short range correlations in low energy scattering, our method can readily be adapted to systematic machine

calculations of scattering of positrons by any atom for which accurate unperturbed atomic wave functions are known. Improvements in accuracy over the present work can be obtained by inclusion of monopole and higher multipole terms.

Application to the more interesting and more important problem of the scattering of electrons by atoms seems possible although some of the difficulties due to exchange have not been completely resolved. The simplest approach would be to symmetrize our wave functions after we have derived the coupled differential equations for the correlation terms, and then to use the symmetrized wave function for determining the scattered amplitude. We feel, however, that a more correct approach is to symmetrize the trial function before inserting it into the variational principle. The resulting equations, however, are so complicated that some simplifications must be introduced before numerical analysis can begin. We have not investigated in detail what simplifications are possible. A resolution of these difficulties would provide a systematic approach for the problem of the scattering of electrons by atoms.

Appendix I

Asymptotic Expansions of G_o, y_1 and v_1

The behavior of the integral

$$\langle g|R_\gamma|h\rangle$$

in the neighborhood of r = R may be written as

$$\text{(I-1)} \quad \langle g|R_\gamma|h\rangle = \frac{1}{r^{\gamma+1}} \int_o^R g(t)h(t)t^\gamma dt + r^\gamma \int_R^\infty \frac{g(t)h(t)}{t^{\gamma+1}}$$

$$+ \frac{1}{r^{\gamma+1}} \int_R^r g(t)h(t)t^\gamma dt + r^\gamma \int_r^R \frac{g(t)h(t)}{t^{\gamma+1}}\, dt.$$

If the last two terms are expanded in a power series around r = R, the zeroth and first order terms vanish. Then we may approximate $\langle g|R_\gamma|h\rangle$ as

$$\text{(I-2)} \quad \langle g|R_\gamma|h\rangle \sim \frac{1}{r^{\gamma+1}} \int_o^R g(t)h(t)t^\gamma dt + r^\gamma \int_R^\infty \frac{g(t)h(t)}{t^{\gamma+1}}\, dt.$$

When R = 0,

$$\text{(I-3)} \quad \langle g|R_\gamma|h\rangle \to r^\gamma \int_o^\infty \frac{g(t)h(t)}{t^{\gamma+1}}\, dt.$$

For small r,

$$\text{(I-4)} \quad V_H = \frac{e^{-2r}}{r}(1 + r) \to \frac{1}{r} - 1.$$

Using (I-3) and (I-4) the equations for y,v, and G may be put in the form

$$(I\text{-}5) \qquad \left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} \pm \frac{2}{r} + \lambda\right] F(r) = 0(r)$$

$$F = v \quad , \ \ell = 1, \text{ upper sign}, \ \lambda = E_y + 2\frac{\langle y_1|\frac{1}{r}|y_1\rangle}{\langle y_1|y_1\rangle}$$

$$F = y \quad , \ \ell = 1, \text{ lower sign}, \ \lambda = E_y + 2\frac{\langle v_1|\frac{1}{r}|v_1\rangle}{\langle v_1|v_1\rangle}$$

$$F = G \quad , \ \ell = 0, \text{ lower sign}, \ \lambda = k^2 + 2.$$

Solving for F by means of a power series

$$(I\text{-}6) \qquad F = \sum c_n r^{n+s}$$

we have the recursion relation,

$$(I\text{-}7) \qquad ((n+s)(n+s-1) - \ell(\ell+1))c_n + 2c_{n-1} + \lambda c_{n-2} = 0, \ n \leq 2$$

F will be regular at the origin if $s = \ell + 1$. With this value the first three coefficients are

$$c_o = \text{const.}$$

$$c_1 = \mp \frac{c_o}{\ell + 1}$$

$$c_2 = \left[\frac{1}{(2\ell+3)(\ell+1)} - \frac{\lambda}{2(2\ell+3)}\right] c_o$$

One must take the inhomogeneity into account in order to calculate c_3. Clearly, in the neighborhood of the origin, the particular integral and the complementary function have the same form. The value of c_o necessary

for the particular integral is obtained by satisfying the boundary conditions at infinity.

In order to find the asymptotic forms of y and G, we note that u and v vanish exponentially for large r. Then, according to (I-2) for large R

$$\langle u|R_1|v\rangle = \frac{1}{r^2}\int_0^R uv\, t\, dt.$$

The asymptotic form of the equation defining y is

$$\left[\frac{d^2}{dr^2} - \frac{2}{r^2} - \frac{2}{r} + E_y + \frac{2}{\langle v|v\rangle}\frac{1}{r}\int_0^R vvdt + \frac{4}{5\langle v|v\rangle}\frac{1}{r^3}\int_0^R vt^2vdt\right]y$$

$$= \frac{2}{\langle v|v\rangle}\frac{1}{\sqrt{3}}\frac{1}{r^2}\int_0^R vtudtG$$

or approximately,

$$\text{(I-9)}\qquad \left[\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{4}{5}\frac{\langle v|t^2|v\rangle}{\langle v|v\rangle\, r^3} + E_y\right]y = \frac{2}{\sqrt{3}}\frac{\langle v|t|u\rangle}{\langle v|v\rangle}\frac{G}{r^2} = \gamma_y\frac{G}{r^2}\,.$$

The equation for G is

$$\text{(I-10)}\qquad \left[\frac{d^2}{dr^2} + k^2\right]G = \frac{2}{\sqrt{3}}\langle u|t|v\rangle\ \frac{y}{r^2} = \gamma_G\frac{y}{r^2}$$

$$\gamma_y = \frac{2}{\sqrt{3}}\ \frac{\langle v|t|u\rangle}{\langle v|v\rangle}$$

$$\gamma_G = \frac{2}{\sqrt{3}}\ \langle u|t|v\rangle.$$

Let

$$G = \sum \frac{\alpha_n}{r^n} \sin(kr) + \cos kr \sum \frac{\beta_n}{r^n} \tag{I-11}$$

$$y = \sum \frac{\delta_n}{r^{n+2}} \sin(kr) + \cos kr \sum \frac{\epsilon_n}{r^{n+2}} . \tag{I-12}$$

Substituting (I-11) and (I-12) into (I-9) and (I-10) leads to the recursive relations

$$(E_y - k^2)\delta_n + k(n+1)\epsilon_{n-1} + (n(n+1) - 2)\delta_{n-2} + \frac{4}{5}\frac{\langle v|t^2|v\rangle}{\langle v|v\rangle}\delta_{n-3} = \gamma_y \alpha_n \tag{I-13}$$

$$(E_y - k^2)\epsilon_n - k(n+1)\delta_{n-1} + (n(n+1) - 2)\epsilon_{n-2} + \frac{4}{5}\frac{\langle v|t^2|v\rangle}{\langle v|v\rangle}\epsilon_{n-3} = \gamma_y \beta_n$$

$$k_n\beta_n + n(n-1)\alpha_{n-1} = \gamma_G \delta_{n-3}$$

$$-k_n\alpha_n + n(n-1)\beta_{n-1} + \gamma_G \epsilon_{n-3}. \tag{I-14}$$

The leading terms in (I-13) are

$$\delta_o = \frac{\gamma_y}{E_y - k^2}\alpha_o = \frac{2}{\sqrt{3}}\frac{\langle v|r|u\rangle}{\left\langle v\left|\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1\right|v\right\rangle}\alpha_o$$

$$\epsilon_o = \frac{2}{\sqrt{3}}\frac{\langle v|r|u\rangle}{\left\langle v\left|\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1\right|v\right\rangle}\beta_o \tag{I-15}$$

Thus,

$$y \to \frac{QG}{r^2}$$

$$(I\text{-}16) \qquad Q = \frac{2}{\sqrt{3}} \frac{\langle v|r|u\rangle}{\left\langle v\left|\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1\right|v\right\rangle} \ .$$

From (I-14) we see that

$$(I\text{-}17) \qquad \beta_1 = \beta_2 = \alpha_{-1} = \alpha_2 = 0.$$

In solving the problem numerically, we assume the normalization $\alpha_o = 1$ so that $\beta_o = \tan \eta$.

When $k = 0$, (I-10) reduces to

$$(I\text{-}18) \qquad \frac{d^2}{dr^2} G = \gamma_G \frac{y}{r^2} \ .$$

The complete homogeneous solution to (I-19) is of the form $\alpha_o r + \alpha_1$. Accordingly, we take

$$G = \sum_n \frac{\alpha_n}{r^{n-1}}$$

$$y = \sum \frac{\delta_n}{r^{n+1}}$$

which, after substitution into (I-18,11), result in

$$(I\text{-}20) \qquad E_y \delta_n + (n(n-1)-2)\delta_{n-2} + \frac{4}{5} \frac{\langle v|t^2|v\rangle}{\langle v|v\rangle} \delta_{n-3} = \gamma_y \alpha_n$$

$$n(n-1)\alpha_n = \gamma_\epsilon \delta_{n-2}.$$

We take $\alpha_o = 1$, so that α_1 is the scattering length. From (I-20), we see that none of the α_n vanish. Thus the particular integral vanishes as $\frac{1}{r}$. When $k \neq 0$, the particular integral vanishes as $\frac{1}{r^3}$. Thus,

$$\frac{\text{Particular Integral}}{\text{Complementary function}} \quad \begin{cases} \frac{1}{r^2}, & k = 0 \\ \\ \frac{1}{r^3}, & k \neq 0 \end{cases}$$

and we see that the polarization plays a larger role for $k = 0$.

We have in general for v

$$\text{(I-21)} \qquad \left[\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} + E_v + \frac{2}{\langle y|y\rangle} \left(\langle y|R_o|y\rangle + \frac{2}{5}\langle y|R_2|y\rangle \right) \right] v$$

$$= \frac{2}{\sqrt{3}} \langle y|R_1|G\rangle u$$

$$u = 2r\, e^{-r}$$

Now

$$r^\gamma \int_R^\infty \frac{y^2}{t^{\gamma+1}}\, dt \sim r^\gamma Q^2 \frac{1}{R^{4+\gamma}} \sim \frac{Q^2}{R^4}$$

$$r \int_R^\infty \frac{yG}{t^2}\, dt \sim r \frac{Q}{R^3} \sim \frac{Q}{R^2} .$$

Thus, for R large, we can approximate (I-21) by

$$\text{(I-22)} \qquad \left[\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{4}{r} + E_v\right]v = \frac{4\, e^{-r}}{\langle y|y\rangle\sqrt{3}}\left[\frac{1}{r}\int_0^R ytG\,dt + r^2\int_R^\infty \frac{yG}{t^2}\,dt\right]$$

$$= \left[\frac{A}{r} + Br^2\right]e^{-r}.$$

There are two particular integrals for v,

$$\text{(I-23)} \qquad v = \left[\sum \lambda_n \frac{1}{r^{n+1}} + \sum \zeta_n \frac{1}{r^{n-2}}\right]e^{-r}$$

which results in the recursion relation.

$$\text{(I-24)} \qquad \begin{aligned} &(E_v + 1)\lambda_n + \left[4 + (n-1)\right]\lambda_{n-1} + \left[(n-1) - 2\right]\lambda_{n-2} = A\delta_{no} \\ &(E_v + 1)\zeta_n + \left[4 + (n-3)\right]\zeta_{n-1} + \left[(n-4)(n-3) - 2\right]\zeta_{n-2} = B\delta_{no} \end{aligned}$$

We keep only the leading terms,

$$\text{(I-25)} \qquad \lambda_o = \frac{4}{\sqrt{3}}\,\frac{\int_o^R yt\,G\,dt}{\left\langle y\left|\frac{d^2}{dr^2} - \frac{2}{r^2} - \frac{2}{r} + k^2\right|y\right\rangle}$$

$$\zeta_o = \frac{4}{\sqrt{3}}\,\frac{\int_R^\infty \frac{yG}{t^2}\,dt}{\left\langle y\left|\frac{d^2}{dr^2} - \frac{2}{r^2} - \frac{2}{r} + k^2\right|y\right\rangle}.$$

We can use this technique to solve

$$\left[\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1\right] v_{AD} = -4r^2 e^{-r}$$

by defining

$$v_{AD} = w\, e^{-r}.$$

Then

$$\left[\frac{d^2}{dr^2} - 2\frac{d}{dr} - \frac{2}{r^2} + \frac{2}{r}\right] w = -4r^2 .$$

Let

$$w = \sum \frac{a_n}{r^{n-s}}$$

which results in

$$\sum_n \frac{2(n-s) + 2}{r^{n-s+1}} + \sum \left((n-s)(n-s+1)-2\right) \frac{a_n}{r^{n-s+2}} = -4r^2 .$$

If $a_o \neq 0$, then $s = 3$ and we have the recursion relation

$$(2n - 6)a_n + \left((n - 4)(n - 3) - 2\right) a_{n-1} = -4\delta_{no}$$

and

$$a_o = +1$$

$$a_1 = 2a_o = 2$$

$$a_2 = 0$$

(I-27) $$v_{AD} = e^{-r} w = \left[a_o r^3 + a_1 r^2\right] = (2r^2 + r^3)e^{-r}.$$

It is interesting to note that, in the case of v_{AD}, the inhomogeneous term goes as r^2e^{-r} and the solution goes as r^3e^{-r}. This results from the fact that the coefficient of r in the exponential is the same as the constant in the operator and is comparable to a resonance effect. In all other cases considered the two numbers are quite different and we have the result that the leading term of the particular integral is given by the inhomogeneity multiplied by some constant.

It is necessary to know the complementary function of (I-22) which is regular at infinity for the numerical work. Thus, we take

$$\left[\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{4}{r} + E_v\right]v^{(2)} = 0$$

$$v^{(2)} \to 0 \qquad r \to \infty$$

E_v is negative for small k so we take

$$v^{(2)} = r^s e^{-\lambda r} z \ , \qquad \lambda = \sqrt{-E_v}$$

Then

$$\left[\frac{d^2}{dr^2} + \left(\frac{2s}{r} - 2\lambda\right)\frac{d}{dr} + \frac{s(s-1)-2}{r^2} + \frac{4-2\lambda s}{r}\right]z = 0$$

Let $s = \frac{2}{\lambda}$ and take z to be of the form

$$z = \sum \frac{b_n}{r^n}$$

which results in the recursion relation

$$2\lambda b_n + \left[n(n-1) + \left(\frac{2}{\lambda}\left(\frac{2}{\lambda} - 1\right) - 2\right) - \frac{4}{\lambda}(n-1)\right] b_{n-1} = 0,$$

and therefore

$$v^{(2)} \rightarrow b_o \, r^{\frac{2}{\sqrt{-E_v}}} \, e^{-\sqrt{-E_v}\, r} \left(1 + \frac{2 - \left(\frac{2}{\lambda}\left(\frac{2}{\lambda} - 1\right)\right)}{2\lambda}\right) .$$

Appendix II

Techniques Used in Numerical Integration

Let us write the equation to be solved in the notation

(II-1) $\mathcal{L}_1 G = f_1 y$

(II-2) $\mathcal{L}_2 v = f_2 u$

(II-3) $\mathcal{L}_3 y = f_3 G$

Since we do not know the boundary conditions on G, y or v, it is necessary to iterate the equations in the hope that the solutions will converge. The interation was started by using v_{AD} for $v^{(o)}$ and G_H for $G^{(o)}$ where

$$\mathcal{L}_1 G_H = 0.$$

The functions $v^{(o)}$ and $G^{(o)}$ were used to solve for $y^{(o)}$; $y^{(o)}$ and $v^{(o)}$ for $G^{(1)}$; $G^{(1)}$ and $y_1^{(o)}$ for $v^{(1)}$ and so forth.

The numerical integration of these equations was performed by means of a difference scheme known as Milnes' Method [14]. This method requires the knowledge of four previous values of the function and their second derivatives in order to step ahead. Let Δ be the interval and suppose we have obtained the values z_i, z_i'', $i = 1,2,3,4$. One makes an estimate of z_5 from

(II-4) $$z_5^{(o)} = 2z_3 - z_1 + 4\Delta^2(z_3'' + \delta^2 z_3''/3)$$

where

(II-5) $$\delta^2 z_i'' = z_{i+1} - 2z_i + z_{i-1}.$$

The second derivative at $i = 5$ can be computed using $z_5^{(o)}$. The corrected value of z_5 is obtained from

(II-6) $$z_5 = -2z_4 + z_3 + \Delta^2(z_4'' + \delta^2 z_4''/12).$$

The multipole integrals

$$\langle z|R_\gamma|w \rangle$$

were carried out by changing the form to read

$$\text{(II-7)} \qquad \langle z|R_\gamma|w\rangle = \frac{1}{r^{\gamma+1}} \int_0^r zwt^\gamma dt - r^\gamma \int_0^r \frac{zw}{t^{\gamma+1}} + r^\gamma \int_0^\infty \frac{zw}{t^{\gamma+1}} dt.$$

The first two terms are integrated from the origin using a four point difference formula. Thus

$$\text{(II-8)} \qquad \int_{x_1}^{x_{i+1}} w(t)dt = \Delta \sum_{j=1}^{4} c_j w_{i-j}$$

$$c_1 = 0.37500$$

$$c_2 = 0.79167$$

$$c_3 = -0.20833$$

$$c_4 = 0.041667$$

The integrations are carried foward to some value R where the functions assume their asymptotic form. The third term in (II-7) may then be evaluated by adding a correction

$$I_c^\gamma(zw) = \int_R^\infty \frac{zw}{t^{\gamma+1}} dt$$

to the integral $\int_0^R \frac{zw}{t^{\gamma+1}} dt$ which has already been computed. Since v and u fall off rapidly, $I_c^\gamma(v,v)$ and $I_c^1(v,u)$ are negligible. $I_c^\gamma(y,y)$ and $I_c^1(y,G)$ are computed by assuming

$$G = \sin(kr) + \tan\eta \cos(kr)$$

$$y = \frac{QG}{r^2}$$

for $r > R$. $I_c^{\gamma}(y,y)$ and $I_c^{1}(y,G)$ can then be integrated by parts a number of times depending on γ. The result is expressed in terms of sine and cosine integrals the values of which must be supplied with the initial data. The definite integrals $\langle w|w \rangle$ are carried out in a similar fashion.

Four values of the function are necessary to initiate the integration. These may be computed from (I-8). The choice of c_o is arbitrary since an error in c_o will have the effect of introducing the homogeneous solution. Thus, suppose we are integrating the equation

(II-9) $$\mathcal{L}w = fz$$

with the homogeneous solution $w^{(1)}$ and $w^{(2)}$ defined by

(II-10) $$\mathcal{L}w^{(1)} = 0$$

$$w^{(1)} = \text{regular at the origin}$$

$$w^{(2)} = \text{regular at infinity.}$$

If we use the polynomial (I-6) to start the integrations, and we choose $c_o = c_o^{(t)}$ we can expect the trial function $w^{(t)}$ to be of the form

(II-11) $$w_f^{(t)} = w + \beta_{1f} w^{(1)} + \beta_{2f} w^{(2)}$$

where w is the desired particular integral with $c_o = c_o^{(c)}$. The coefficient, β_{2f}, arises from having truncated (I-6) and can be shown to be negligible. The coefficient, β_{1f}, is proportional to the difference

$c_o^{(t)} - c_o^{(c)}$. It is also possible to start the integration by means of the asymptotic forms (I-12) , (I-23) and this was done in the v integration. In this case one obtains

$$w_b^{(t)} = w + \beta_{1b} w^{(1)} + \beta_{2b} w^{(2)} .$$

In this case, β_{1b} and β_{2b} are results of truncation errors. β_{1b} is usually less than β_{2b} and since $w^{(1)}$ decreases exponentially with decreasing r, $\beta_{1b} w^{(1)}$ becomes smaller as the integration proceeds. (The same holds true of $\beta_{2f} w^{(2)}$ in (II-11).) In order to obtain the particular integral w, we require that

$$w_f^{(t)} + \beta_f w^{(1)} = w_b^{(t)} + \beta_b w^{(2)} = w . \qquad \text{(II-12)}$$

Requiring (II-12) to be satisfied at two values of the argument w, we are able to solve for β_f and β_b and consequently w. An alternative procedure which was carried out for y and G is to carry out the forward integration until the cutoff value R is reached. One then matches $w_f^{(t)}$ with the asymptotic form (I-11) for the G integration and (I-12) for the y integration.

In determining the value of β_f for $G_f^{(t)}$, we set $\alpha_o = 1$, $\beta_o = 0$ in (I-11) so that

$$G_{AS} = \sin kr \sum \frac{\alpha_n}{r^n} + \cos kr \sum \frac{\beta_n}{r^n} . \qquad \text{(II-13)}$$

The matching equations are then

$$G_f^{(t)} + \beta_f G^{(1)} = G_{AS} + \tan \eta \cos kr. \qquad \text{(II-14)}$$

Requiring (II-14) to hold at two points is sufficient to determine β_f and tan η.

The value of β_f for $y_f^{(t)}$ is obtained by setting β_o = tan η and defining y_{AS} as the quotient of (I-12) divided by

$$Q = \frac{2}{\sqrt{3}} \frac{\langle v|r|u\rangle}{\left\langle v\left|\frac{d^2}{dr^2} - \frac{2}{r^2} + \frac{2}{r} - 1\right|v\right\rangle} .$$

We then require

$$y_f^{(t)} + \beta_f y^{(1)} = Q_N y_{AS} . \qquad \text{(II-15)}$$

Again, requiring (II-15) to hold at two points is sufficient to determine Q_N and β_f. Strictly speaking, Q_N should equal Q and it should be possible to obtain β_f by matching at a single point. In practice, it is found that the asymptotic series defining y does not give sufficient accuracy at the values of R which were chosen. A value of Q_N slightly different from Q will then give a better fit to the assumed asymptotic form.

The value of the cutoff radius, R, is limited by the fact that $y^{(1)} \to \exp\left[+\sqrt{-E_y}\ r\right]$ and that, for small k, E_y is negative. If one is working to an accuracy of n significant figures, and $\exp\left[\sqrt{-E_y}\ R\right]$ is greater than 10^n, then $y_f^{(t)} = \beta_f y^{(1)}$ to n significant figures. As typical figures, let R = 15, Q = 1/2, E_y = -1

$$y \sim \frac{Q}{R^2}\ \frac{1}{2} \cdot 4 \times 10^{-3} = 2 \times 10^{-2}$$

$$y^{(1)} \sim e^{15} \sim 3 \times 10^{6} .$$

Thus, y is contained in the last significant figure of $y_f^{(t)}$ assuming 8 significant figures. The best possible $c_o^{(t)}$ must be in error in the 9^{th} significant figure and therefore gives a β_{lf} of the order of 10^{-8}. The best β_{lf} which occurred was of the order of 10^{-6} so that y is reduced to 6 significant figures. Further reduction in accuracy arises from integration errors. Thus, R = 15 is about as far out as one can take the cutoff radius.

The iterative process was speeded up by taking a linear combination of the input and output values of G. Thus, if $G_I^{(i)}$ was used to compute v and y and these functions, $v_I^{(i)}$ and $y_I^{(i)}$, were used to compute $G_o^{(i)}$, then

$$G_I^{(i+1)} = + G_o^{(i)}\lambda + G_I^{(i)}(1 - \lambda)$$

$$= G_I^{(i)} + \lambda(G_o^{(i)} - G_I^{(i)})$$

where $G_I^{(i+1)}$ is the function used in the next round of iterations. The fastest convergence was found for

$$\lambda = 1.2 .$$

Convergence was also aided by renormalizing v after each iteration. Strictly speaking, this is not necessary since the product vy is independent of the normalizing constant. On the other hand, the $c_o^{(c)}$'s do depend on the normalization and will be improved on each round of integration if the normalization of each function is kept constant.

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